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Theory of the hole subband dispersion in strained and unstrained quantum wells

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We use the spherical model to derive simple selection rules for the mixing and dispersion of light- and heavy-hole subbands in both strained and unstrained quantum-well systems. The valence-subband structure of such systems can display surprising features with, for instance, the highest hole band being light-hole-like in the well plane near the zone center and strongly nonparabolic at larger wave vectors. We use the infinite square-well potential to show how these and other unintuitive features in the valence-subband dispersion can be understood in terms of interactions between the two highest heavy-hole subbands and the highest light-hole subband. Finally, we give guidelines for optimizing the valence-subband structure for specific applications: first to achieve maximal light-hole behavior and second for a highly nonparabolic band structure for nonlinear devices.

There is an increasing interest in the valence-subband dispersion of quantum wells and superlattices. It has been shown experimentally[1] that the highest hole band in a strained-layer superlattice can have an anomalously low effective mass. Theoretical calculations show the highest hole band to have a low effective mass in both strained and unstrained systems[2-4] and, in addition, show a highly nonparabolic subband dispersion near the valence-band maximum. This low effective mass and nonparabolic dispersion have many potentially significant device applications. The low effective mass is of potential benefit in fast complementary logic devices[5] and for reducing threshold current and increasing T_0 in semiconductor injection lasers,[6] while the strong nonparabolicity offers the potential of large nonlinearities for optical switching devices.[3] In this Rapid Communication we examine the origins of this novel behavior and show how it can be explained using effective-mass theory and simple selection rules.

We use the Luttinger-Kohn (LK) Hamiltonian[7] in the spin $-\frac{3}{2}$ basis, and a spherical model[8] for the band structure. This model ignores the conduction band and the spin-split-off band and treats the highest valence bands as isotropic parabolas with dispersion relations given by $E_-(k)=-(\gamma_1-2\bar{\gamma})k^2$ for the doubly degenerate heavy-hole band and $E_+(k)=-(\gamma_1+2\bar{\gamma})k^2$ for the doubly degenerate light-hole band, with the valence-band maximum taken as the zero of energy. We take $\hbar=2m=1$, with the Bohr radius as the unit of length and energies in rydbergs. The effective masses for the heavy- and light-hole bands are then $m_h^*=(\gamma_1-2\bar{\gamma})^{-1}$ and $m_l^*=(\gamma_1+2\bar{\gamma})^{-1}$, respectively. The true bands are of course anisotropic, but the anisotropy factor, given by $(\gamma_3-\gamma_2)/\gamma_3$ in the LK Hamiltonian, is generally only of order 10%–25% for the III-V systems of interest[9] and can be ignored. We examine the dispersion of this Hamiltonian first in a strained bulk semiconductor, where we recover the results of Pikus and Bir.[10] We then consider a general quantum well. We derive selection rules for hole-band mixing away from Γ, the two-dimensional Brillouin-zone center, and then apply these selection rules to the case of a strained infinite square-well potential. Finally, we show that the important features in the band structure can be explained using a small subset of the selection rules and give general guidelines for optimal band structures for specific applications.

In the spherical model, the LK Hamiltonian for a bulk strained semiconductor can be decoupled into two equivalent 2×2 matrices. We choose the z axis as the quantization axis for angular momenta and apply a uniform axial strain along the x axis. The strain splits the degeneracy of the valence-band maximum at Γ. The band structure is symmetric about the y-z plane so we can set $k_z=0$ without loss of generality. The Hamiltonian then takes the form

$$H(k_x,k_y)=\begin{pmatrix} E_v+\delta-(\gamma_1+\bar{\gamma})(k_x^2+k_y^2) & 3^{1/2}[\bar{\gamma}(k_x-ik_y)^2-\delta] \\ 3^{1/2}[\bar{\gamma}(k_x+ik_y)^2-\delta] & E_v-\delta-(\gamma_1-\bar{\gamma})(k_x^2+k_y^2) \end{pmatrix}, \tag{1}$$

where E_v is the mean energy of the valence states at Γ, and 4δ is the strain-induced splitting of the valence-band maximum. The resulting band structure is anisotropic. The bands along the strain direction ($k_y=0$) have the same dependence on k_x as in an unstrained crystal with

$$E_+(k_x)=E_v+2\delta-(\gamma_1+2\bar{\gamma})k_x^2 ,$$
$$E_-(k_x)=E_v-2\delta-(\gamma_1-2\bar{\gamma})k_x^2 .$$

At small k_y the bands perpendicular to the strain axis are given by

$$E_+(k_y)=E_v+2\delta-(\gamma_1-\bar{\gamma})k_y^2 ,$$
$$E_-(k_y)=E_v-2\delta-(\gamma_1+\bar{\gamma})k_y^2 .$$

Thus the band which is heavy along the strain direction [$m^*=(\gamma_1-2\bar{\gamma})^{-1}$] is comparatively light perpendicular

to that direction [$m^* = (\gamma_1 + \bar{\gamma})^{-1}$] and vice versa. This anisotropy follows from the lifting of the degeneracy of the valence-band maximum and can be understood via $\mathbf{k}\cdot\mathbf{p}$ theory.[10,11]

For quantum-well structures, we choose the growth direction along the x axis. The mean valence-band maximum energy and strain-induced splitting now vary along the growth direction as $E_v(x)$ and $\delta(x)$, respectively. We replace k_x by $-i\partial/\partial x$ and rewrite the Hamiltonian as the sum of two terms, the first of which $H_0(-i\partial/\partial x, 0)$ is the Hamiltonian at the center of the two-dimensional Brillouin zone, while the second term $H_1(-i\partial/\partial x, k_y)$ includes all terms involving k_y, the wave vector in the well plane. For a potential without a plane of inversion perpendicular to the x direction, the two LK Hamiltonians are no longer equivalent[12] and we must replace k_y by $-k_y$ in the second 2×2 matrix.

The Hamiltonian H_0 can always be decoupled to give states at the zone center whose character is purely light-hole-like or heavy-hole-like when viewed along the growth direction. The eigenfunctions of H_0 with energies $E_m^{\pm}$ are $\phi_m^+ = V^+ f_m^+(x)$ for light holes and $\phi_m^- = V^- f_m^-(x)$ for heavy holes, where $V^+ = \frac{1}{2}\begin{pmatrix}-\sqrt{3}\\ 1\end{pmatrix}$ and $V^- = \frac{1}{2}\begin{pmatrix}1\\ \sqrt{3}\end{pmatrix}$ and $f_m^{\pm}$ are solutions of the Schrödinger equation

$$(\gamma_1 \pm 2\bar{\gamma})\partial^2 f_m^{\pm}/\partial x^2 + [E_v(x) \pm 2\delta(x)] f_m^{\pm}(x) = E_m^{\pm} f_m^{\pm}(x) .$$

The normalization chosen is such that $\langle f_m^{\pm} | f_m^{\pm}\rangle = 1$.

We calculate the bands away from Γ by examining how H_1 mixes the zone-center states. The interactions between zone-center states are as follows:

$$\text{(i)}\quad \langle \phi_m^{\pm} | H_1 | \phi_m^{\pm}\rangle = -(\gamma_1 \mp \bar{\gamma})k^2 . \tag{2}$$

This contribution to the dispersion in the well plane is identical to the dispersion found perpendicular to the strain axis in a strained bulk material. It is due to the lifting of the degeneracy of the valence states and we shall refer to it as the splitting-induced dispersion.

$$\text{(ii)}\quad \langle \phi_m^{\pm} | H_1 | \phi_n^{\pm}\rangle = 0, \text{ if } m \neq n . \tag{3}$$

Light-hole states do not interact directly with other light-hole states nor do heavy-hole states interact directly with other heavy-hole states.

$$\text{(iii)}\quad \langle \phi_m^{\pm} | H_1 | \phi_n^{\mp}\rangle = \pm 2\sqrt{3}\bar{\gamma}k\langle f_m^{\pm} | \partial/\partial x | f_n^{\mp}\rangle + \sqrt{3}\bar{\gamma}k^2\langle f_m^{\pm} | f_n^{\mp}\rangle . \tag{4}$$

In a general potential, interactions of order k and of order k^2 are possible between all light-hole states $|\phi_m^+\rangle$ and all heavy-hole states $|\phi_n^-\rangle$. In a symmetric potential where the eigenstates $|\phi_m^{\pm}\rangle$ are of even (odd) parity for m even (odd) the first term in (4) vanishes when m and n are of the same parity and the second term vanishes when m and n are of different parity. For a symmetric potential, we can therefore say the following. (iv) There is an interaction of order k between light-hole state $|\phi_m^+\rangle$ and heavy-hole state $|\phi_n^-\rangle$ when $m+n$ is odd. (v) There can be an interaction of order k^2 between light-hole state $|\phi_m^+\rangle$ and heavy-hole state $|\phi_n^-\rangle$ when $m+n$ is even. This interaction is zero in an infinite square well unless $m=n$, so it is expected to be small in the general case for $m \neq n$.

Use of these selection rules allows us to understand the hitherto nonintuitive features of the valence-band dispersion in quantum-well systems. As an example, we consider the band structure of an infinite square well with uniform strain δ. The zone-center states are at $E_n^{\pm} = -(\gamma_1 \pm 2\bar{\gamma}) \times (n\pi/L)^2 \pm 2\delta$, where L is the well width and the envelope wave functions are given by $f_m^{\pm}(x) = (2/L)^{1/2} \times \sin(m\pi x/L)$. The interaction between ϕ_m^+ and ϕ_n^- is given by Eq. (4) as

$$\langle \phi_m^+ | H_1 | \phi_n^-\rangle = [1+(-1)^{m+n+1}]\frac{4\sqrt{3}\bar{\gamma}k}{L}\frac{mn}{m^2-n^2} + \sqrt{3}\bar{\gamma}k^2\delta_{mn} . \tag{5}$$

The band effective masses at the zone center can then be calculated using second-order perturbation theory and are given by

$$\frac{1}{m^*_{\pm n}} = -(\gamma_1 \mp \bar{\gamma}) + \sum_{\substack{m \\ (m+n \text{ odd})}} \frac{192\bar{\gamma}^2/L^2\left(\frac{mn}{m^2-n^2}\right)^2}{E_n^{\pm} - E_m^{\mp}} . \tag{6}$$

The infinite sum in (6) can be calculated using the Sommerfeld-Watson transformation,[13] and it can be shown that the effective mass for $\delta = 0$ is identical to that derived by Nedorezov:[14]

$$\frac{1}{m^*_{\pm n}} = -(\gamma_1 \pm 2\bar{\gamma})\left\{\frac{3[\cos(n\pi\omega^{\pm}) + (-1)^{n+1}]}{(n\pi\omega^{\pm})\sin(n\pi\omega^{\pm})} + 1\right\} , \tag{7}$$

where $\omega^{\pm} = [(\gamma_1 \pm 2\bar{\gamma})/(\gamma_1 \mp 2\bar{\gamma})]^{1/2}$. Equation (6) indicates the relative importance of different interactions in determining the dispersion at small k. For the highest hole band with $\gamma_1 = 6.85$ and $\bar{\gamma} = 2.58$ (values appropriate to GaAs[3]) the splitting-induced dispersion gives an effective mass within 16% of the exact value of equation (7), while including the interaction with the second light-hole band reduces the error in calculated effective mass to less than 1%.

We propose that the valence-subband dispersion for most structures can be modeled by considering only the interactions between the highest light-hole band LH1 and the two highest heavy-hole bands HH1 and HH2. We illustrate this in Fig. 1, where we present the band structure of an unstrained GaAs infinite square well with $L = 100$ Å, calculated (a) exactly using the spherical model and (b) considering only the splitting-induced dispersion $-(\gamma_1 \mp \bar{\gamma})k^2$ and the interactions between LH1 and HH1, $3^{1/2}\bar{\gamma}k^2$, and between LH1 and HH2, $(16/3^{1/2})\bar{\gamma}k/L$. Figures 1(c) and 1(d) show the equivalent results for $\delta = 6$ meV. The main features in the exact results are reproduced in Figs. 1(b) and 1(d). In particular, the initial anomalous dispersion of the LH1 band is due to the strong interaction between LH1 and HH2.

Finally, we can examine the character of the wave functions with increasing k. This is illustrated in Fig. 2 for the

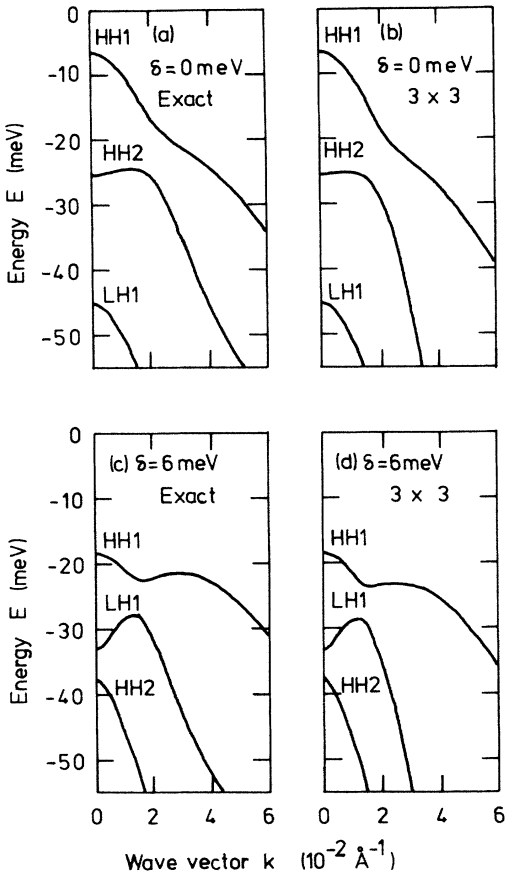

FIG. 1. Valence-subband structure of a 100-Å GaAs quantum well with (a) and (b) $\delta=0$ and (c) and (d) $\delta=6$ meV. (a) and (c) are the exact bands in the spherical model, as derived by Chang (Ref. 3), while (b) and (d) are calculated by considering the interactions between the three highest bands only. The zero of energy is taken as the mean of the bulk light- and heavy-hole band edges.

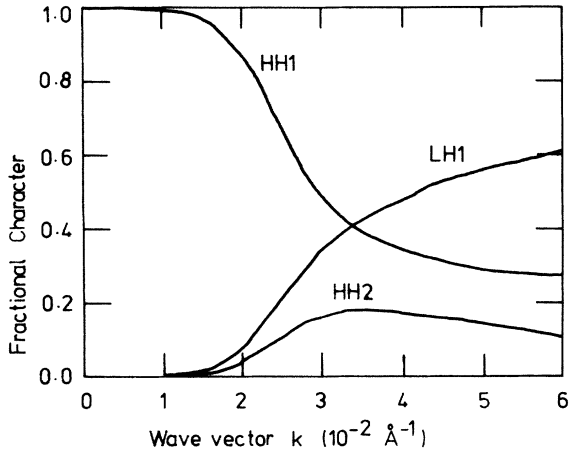

FIG. 2. Character of highest hole band as a function of k. At small k, the wave function is heavy perpendicular to the well plane. At large k, the wave function tends towards 25% HH1 character and 75% LH1 character, appropriate to a state which is heavy in the well plane. Significant band mixing occurs at intermediate k. The contribution from bands other than HH1, HH2, and LH1 never exceeds 5% in total and is omitted from the figure.

highest hole band HH1 for $\delta=0$. The wave function at small k describes a state with heavy-hole character perpendicular to the well. At large k the interactions of order k^2 are dominant, and we approach a state with 25% HH1 character and 75% LH1 character, i.e., a state with heavy-hole character in the well plane. Strong mixing occurs in the intermediate-k region as the state changes over from being heavy perpendicular to the well direction to being heavy in the well plane.

We draw the following conclusions concerning the subband dispersion in strained and unstrained quantum wells.

(1) The highest heavy-hole band HH1 always has a low effective mass for small wave vector k parallel to the well plane. The effective mass will always be larger than that found in a strained bulk semiconductor perpendicular to the strain direction. This increase in effective mass is due to interactions with the light-hole bound states and valence-band resonances.

(2) For complementary logic applications[5] we need to maximize the light-hole behavior at the valence-band edge. This can be achieved by maximizing the splitting between the highest heavy-hole band HH1 and the next subband HH2 or LH2. A large splitting is expected in narrow wells with a substantial valence-band offset between the well and barrier regions so GaAs-AlAs may be a good complementary logic system. The HH1-LH1 splitting can be further enhanced by a built-in biaxial compression in the wells, as in GaAs-InAs.

(3) The most important interaction for a nonparabolic band structure is that of order k between LH1 and HH2. The second highest hole band will have an upwards dispersion (electronlike effective mass) when the LH1 energy is close to or equals the HH2 energy. This condition can always be met in an unstrained quantum-well system for which $m_h^* > 4m_l^*$. For wide wells HH2 then lies above LH1. In sufficiently thin wells, only one light and one heavy bound state are expected, so LH1 must rise above HH2 at some intermediate well width. The inclusion of strain gives an extra degree of freedom to specify the energy splitting between HH1 and HH2 at which the crossover occurs.

(4) For a well with built-in biaxial tension, e.g., as in AlSb-GaSb, LH1 can become the highest hole band. In this case the highest valence band will be heavy in the well plane even at small k. In exceptional circumstances it may even be possible to get an upward dispersion (electronlike effective mass) at the zone center.

(5) We note that the "heavy"-hole effective mass for two-dimensional excitons will be the effective mass in the well plane averaged over a small region of k space near the zone center. This averaged effective mass will depend strongly on the band dispersion near Γ, and for sufficiently large splitting between HH1 and the next highest band should approach the band-edge effective mass given by Eq. (6) and (7).

(6) Finally, as $\gamma_1=\frac{1}{2}(1/m_l^*+1/m_h^*)$ and $\bar{\gamma}=\frac{1}{4}(1/m_l^*$

$-1/m_h^*$), $\bar{\gamma}$ will be largest in materials with a small light-hole effective mass m_l^*. As most of the interactions and effects described here depend on $\bar{\gamma}$, the most significant effects may be found in materials with a low effective mass, such as InAs or even InSb, especially if a barrier material can be found to give deep valence-band confinement wells. The expressions describing intersubband interactions here were calculated assuming infinitely deep confinement wells, but the method can be readily extended to finite square wells or, indeed, wells of arbitrary shape.

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